



## Yasuda-Shedlovsky Result

Sample name: **CS000198**  
Assay name: **pH-metric psKa**  
Assay ID: **11I-14009**  
Filename: **E:\T3 DATA\1109\11I-14009\_CS000198\_pH-metric psKa.t3r**

Experiment start time: **14/09/2011 17:17:30**  
Analyst:  
Instrument ID: **T311042**

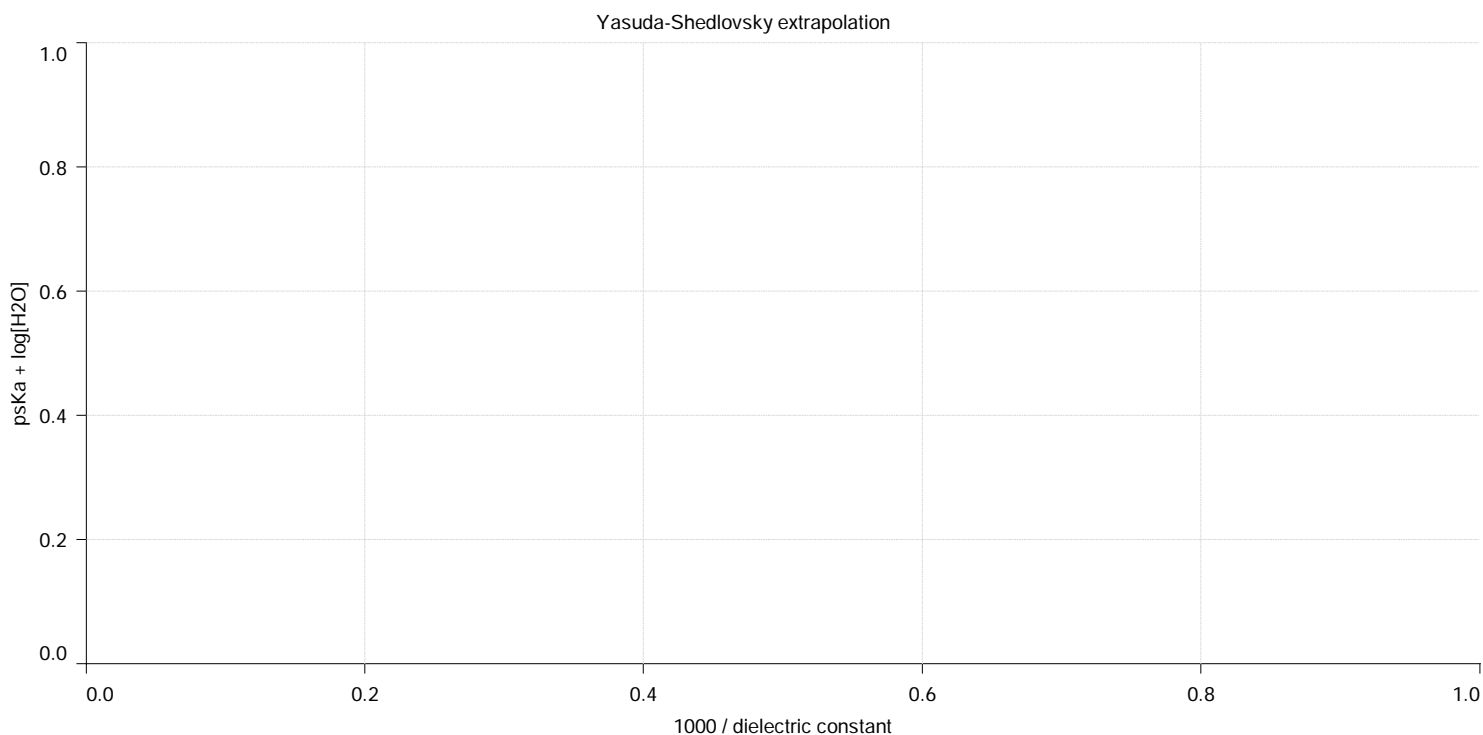
### Yasuda-Shedlovsky result

Extrapolation type pKa 0% SD Intercept Slope R<sup>2</sup> Ionic strength Temperature

### Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H <sub>2</sub> O]	Ionic strength	Temperature
11I-14009 Points 60 to 99	28.36 %	Up	pH-metric	76.0	40.6 M	0.194 M	28.2°C
11I-14009 Points 33 to 59	36.41 %	Up	pH-metric	75.5	36.3 M	0.189 M	27.6°C
11I-14009 Points 3 to 32	46.44 %	Up	pH-metric	74.6	30.9 M	0.177 M	26.8°C

### Graphs



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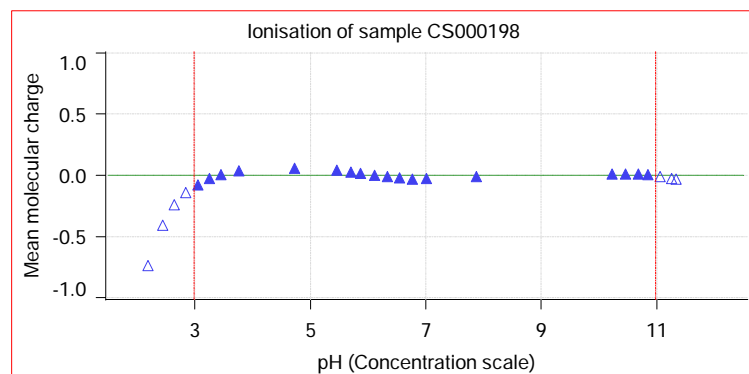
Experiment start time: **14/09/2011 17:17:30**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 1 of 3 11I-14009 Points 3 to 32

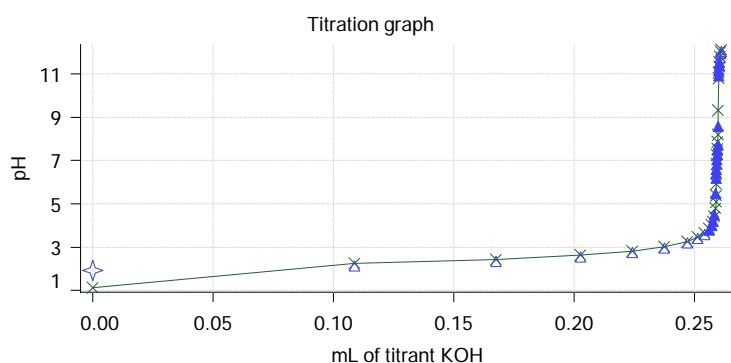
### Sample

 CS000198 concentration factor 0.720

### Sample graphs



### Other graphs



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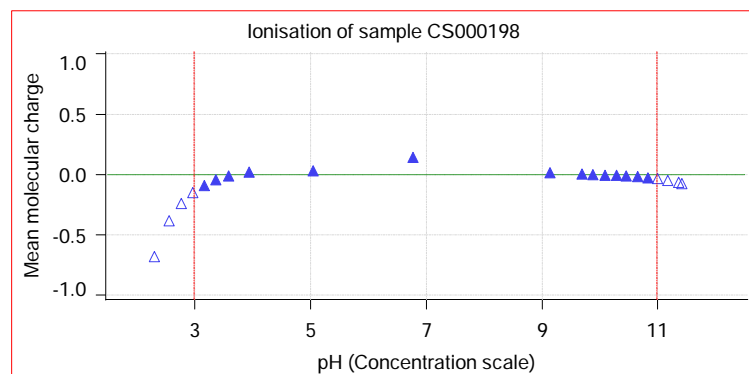
Experiment start time: **14/09/2011 17:17:30**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 2 of 3 11I-14009 Points 33 to 59

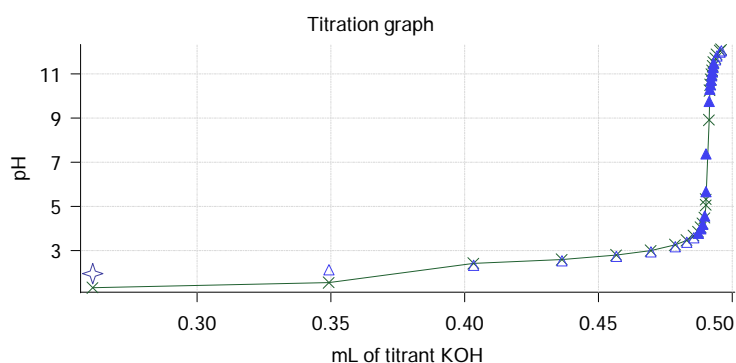
### Sample

 CS000198 concentration factor 0.819

### Sample graphs



### Other graphs



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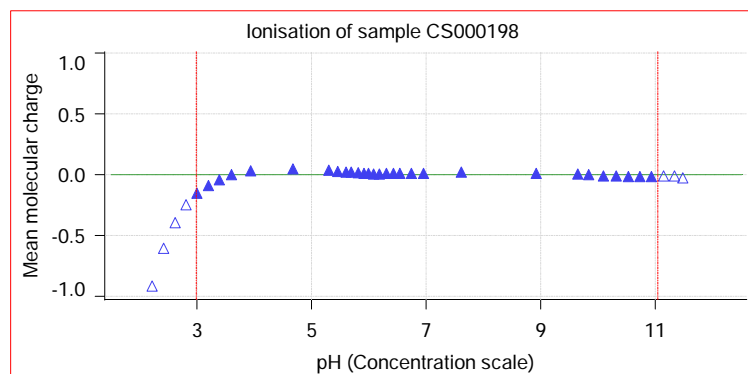
Experiment start time: **14/09/2011 17:17:30**  
 Analyst:  
 Instrument ID: **T311042**

## pH-metric psKa Titration 3 of 3 11I-14009 Points 60 to 99

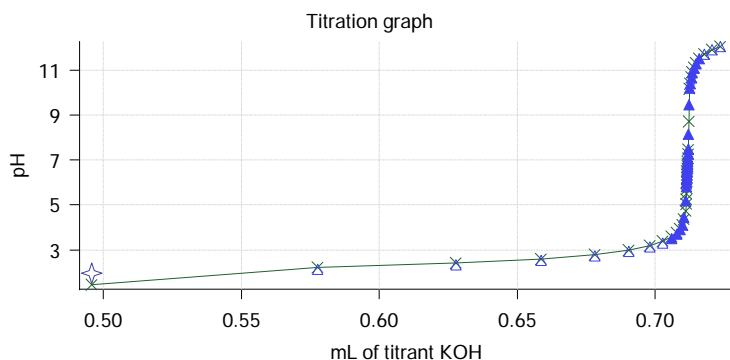
### Sample

 CS000198 concentration factor 0.868

### Sample graphs



### Other graphs



### Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000198		
Sample by	Weight		
Sample weight	0.000940 g		
Formula weight	278.33 g/mol		
Solubility	Unknown		
Molecular weight	Unknown		
Individual pKa ionic environments	No		
Number of pKas	0		
logP (neutral X)	-10.00		